Thermodynamics and Mantle Convection: The role during secular evolution

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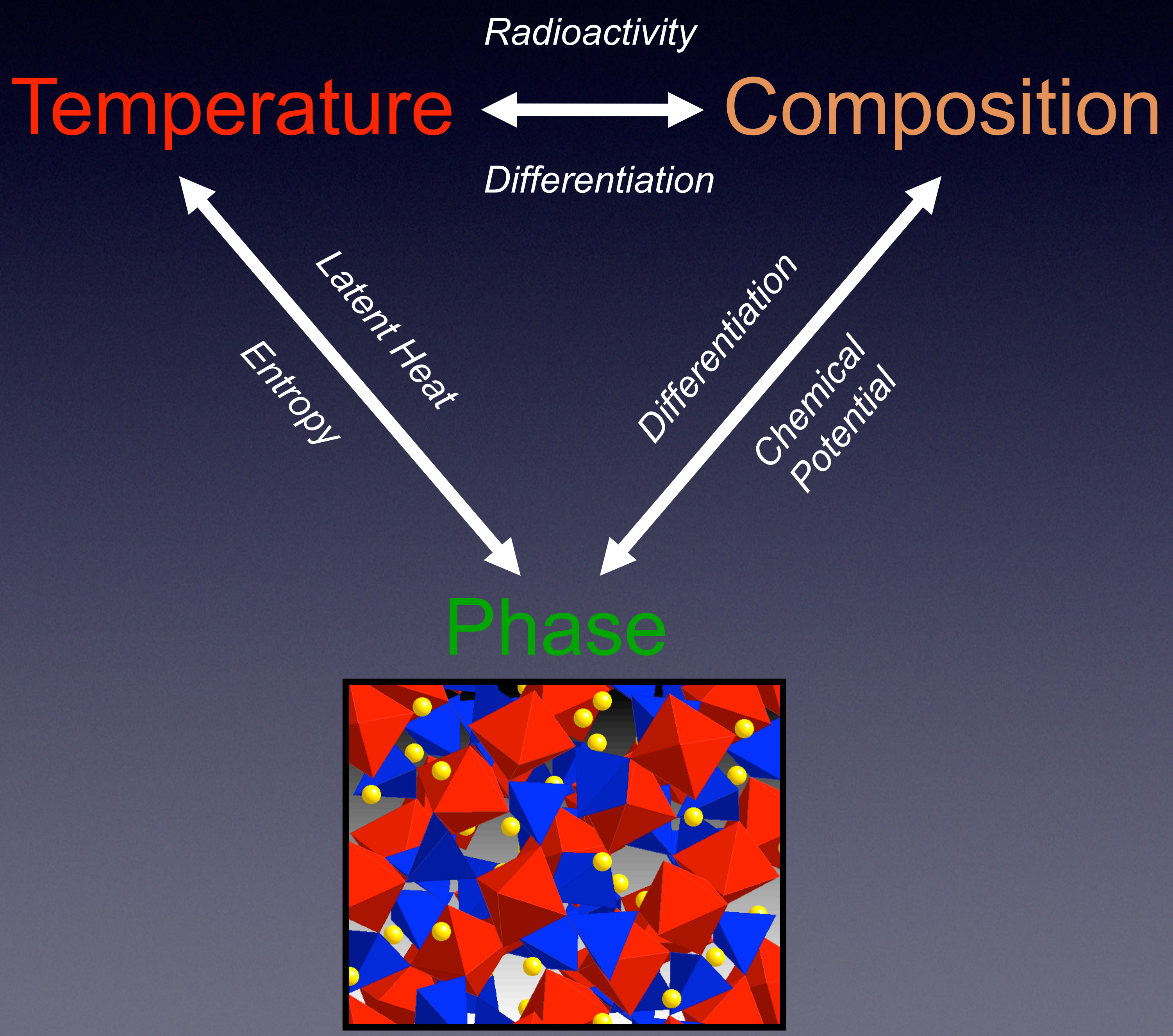
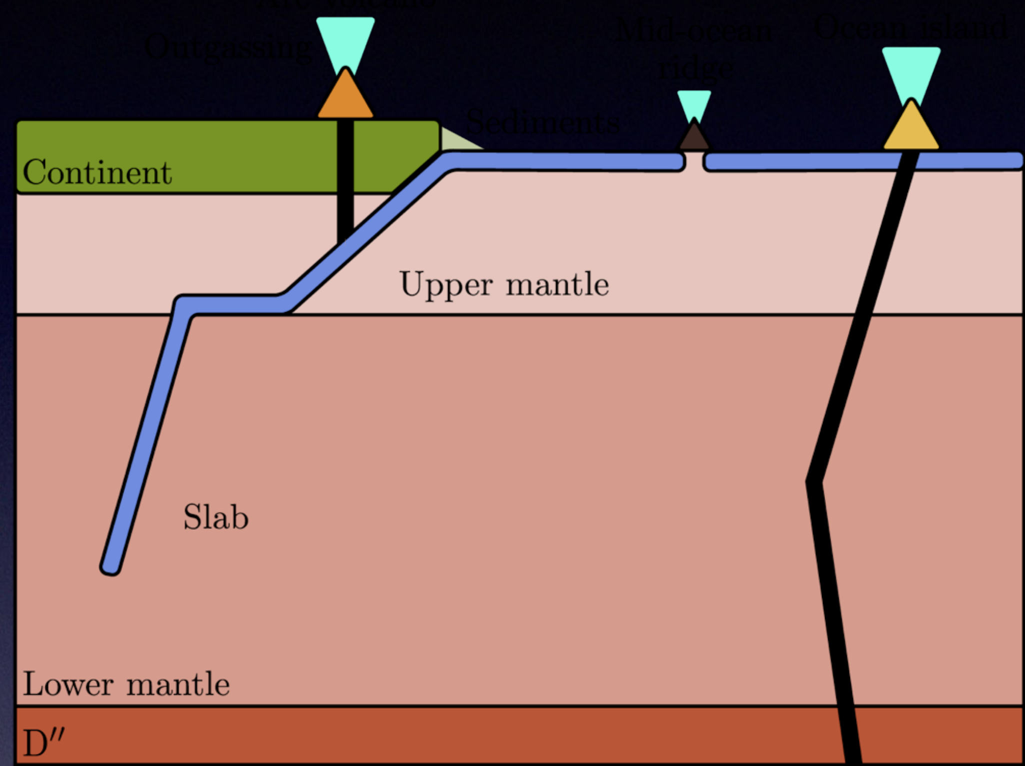
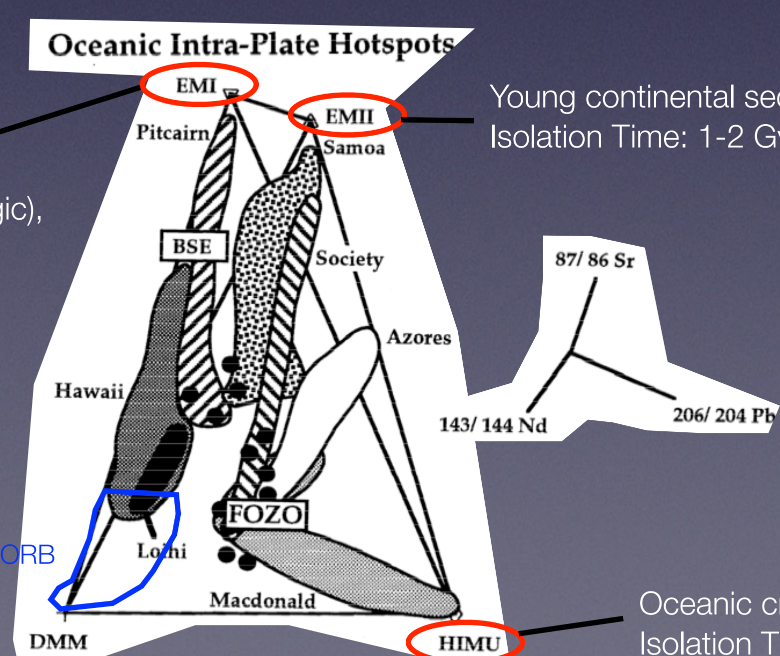
from space to core
earthsciences
UCL

Origin of Heterogeneity



Preservation of Heterogeneity





Young continental sediments
Isolation Time: 1-2 Gyr

Sediments (ancient continental, pelagic), continental lithosphere
Isolation Time: 1-2 Gyr

Oceanic crust
Isolation Time: 2 Gyr

Hauri *et al.* 1994
Hart *et al.* 1992

FT Estimates: Hofmann 1997

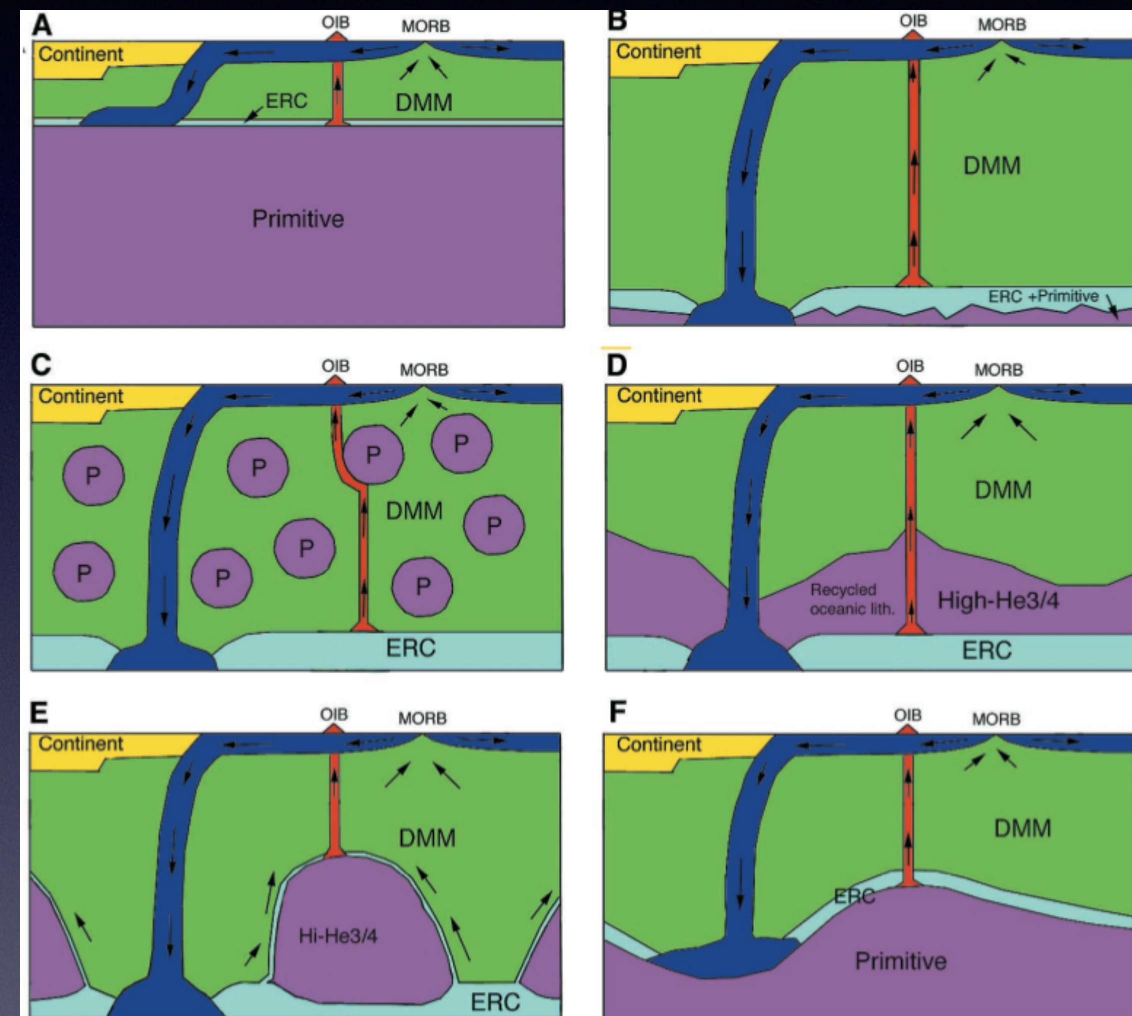
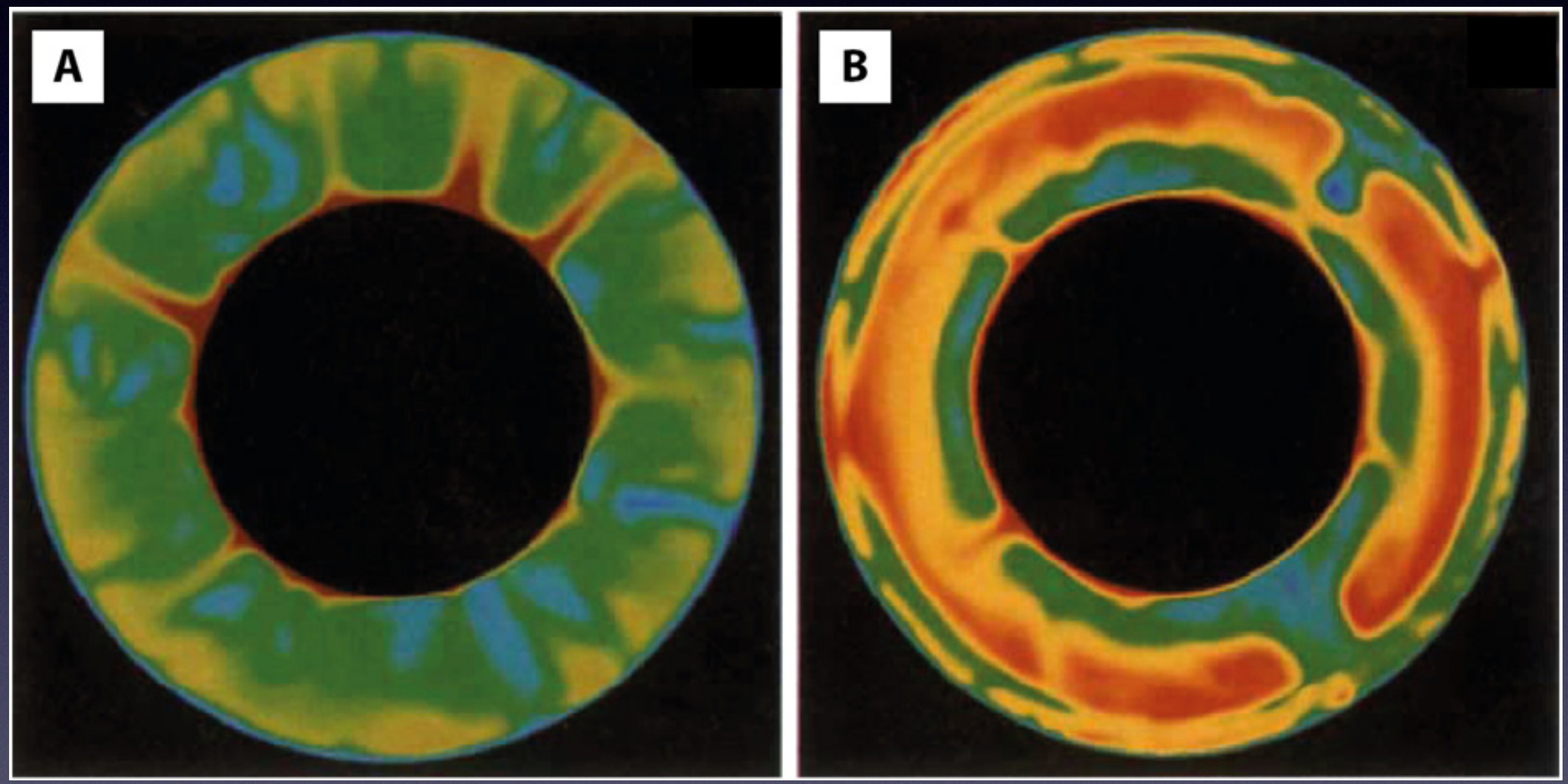


Fig. 2. Some possible locations of mantle reservoirs and relationship to mantle dynamics. Convective features: blue, oceanic plates/slabs; red, hot plumes. Geochemical reservoirs: dark green, DMM; purple, high $^3He/^4He$ ("primitive"); light green, enriched recycled crust (ERC). **(A)** Typical geochemical model layered at 660 km depth (*7*). **(B)** Typical geodynamical model: homogeneous except for some mixture of ERC and primitive material at the base. **(C)** Primitive blob model (*71*) with added ERC layer. **(D)** Complete recycling model (*83, 84*). **(E)** Primitive piles model [developed from (*85*)]. **(F)** Deep primitive layer (*86*).

Tackley 2000

Layered Convection



Tackley 1993

Fig. 5. Cross-sectional slices of the superabiabatic temperature field predicted by one of the earliest 3D global-scale, isoviscous mantle convection simulations. (A) Whole-mantle convection obtained without phase changes switches to (B) intermittent layered convection when adding the post-spinel transition with a strongly negative Clapeyron slope (−4 MPa/K). Scale range from −780 K to +220 K and from −1050 K to +350 K in panels A and B, respectively. From (Tackley et al., 1993).

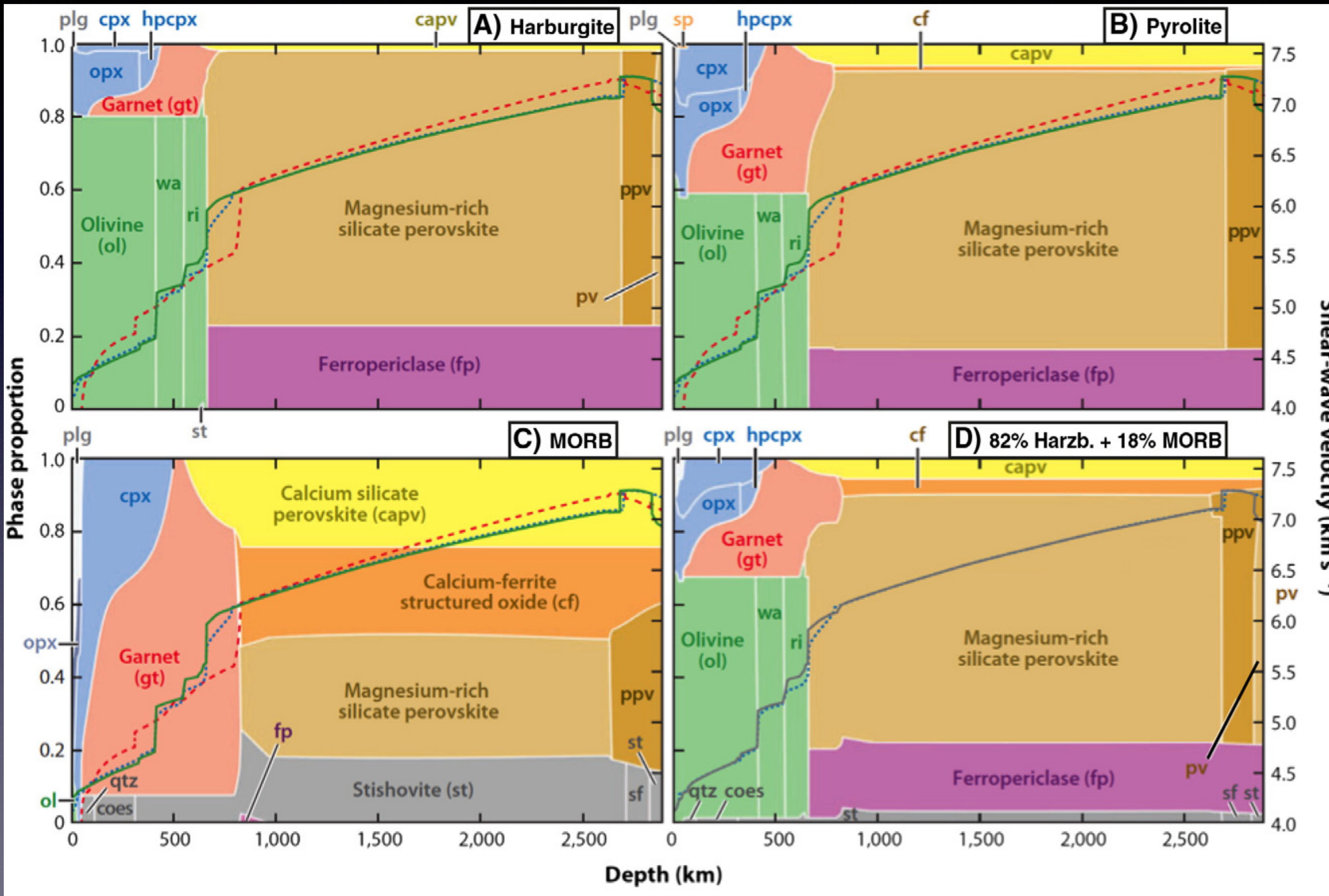
Phase Transitions and Convection

Faccenda and Dal Zilio 2016

$$
\begin{aligned}
\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) - \nabla\cdot k\nabla T = \rho H \\
&+ 2\eta\left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{1}\right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{1}\right) \\
&+ \alpha T\left(\mathbf{u}\cdot\nabla p\right) \\
&+ \rho T\Delta S\left(\frac{\partial X}{\partial t} + \mathbf{u}\cdot\nabla X\right)
\end{aligned}
$$

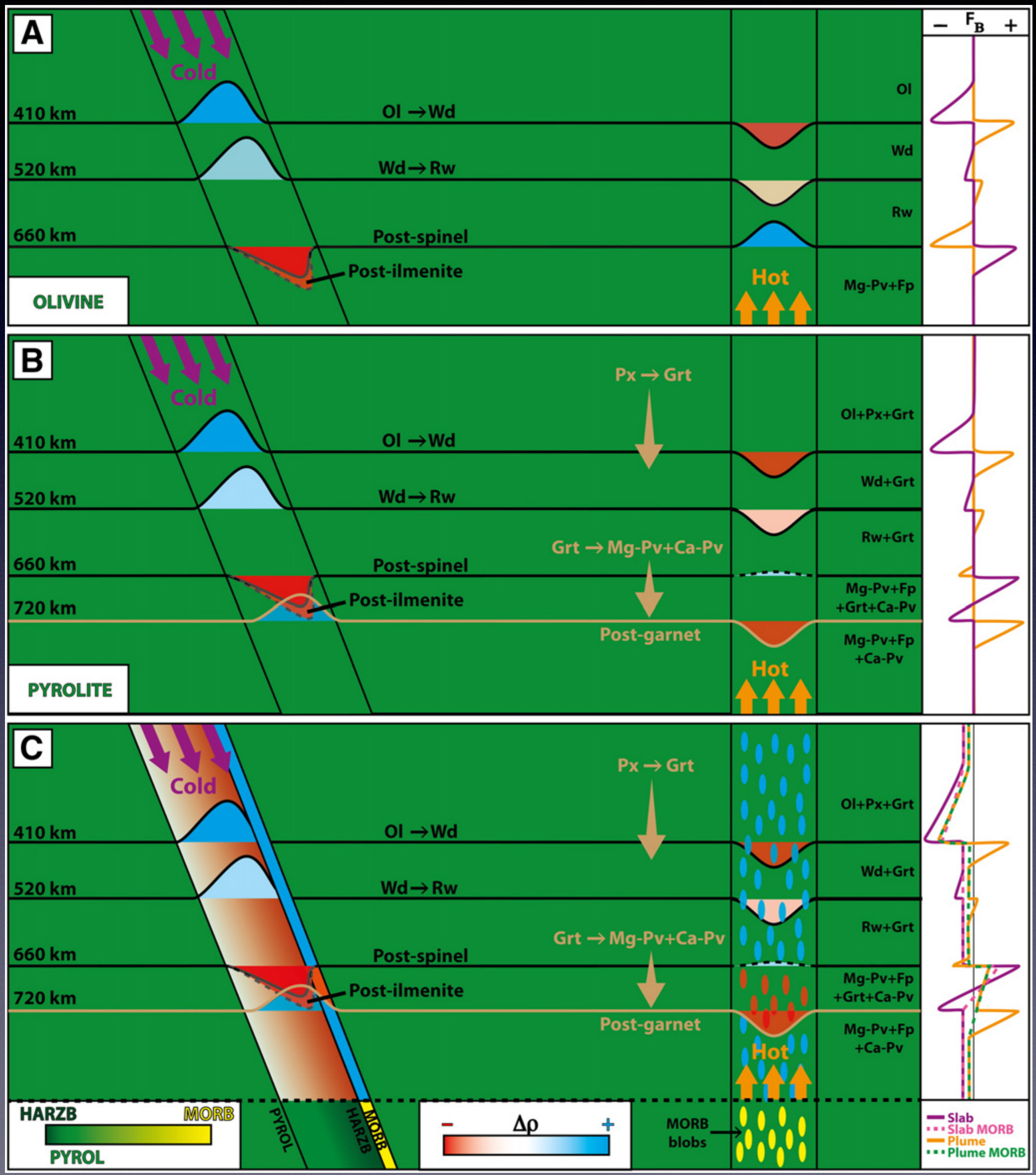
Aspect Manual 2016

Mantle is multiphase

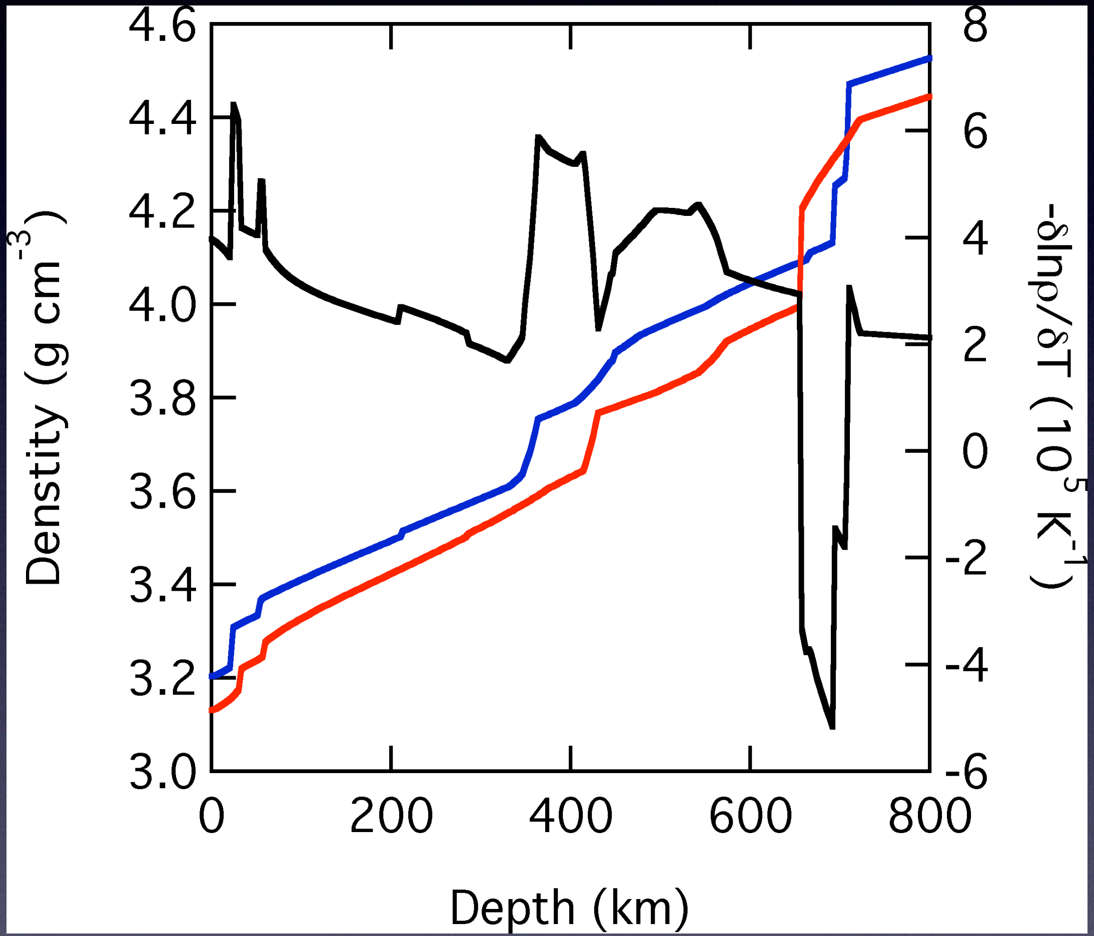


Stixrude and Lithgow-Bertelloni 2012 (AREPS)

Phase Transitions and Dynamics



Faccenda and Dal Zilio 2016

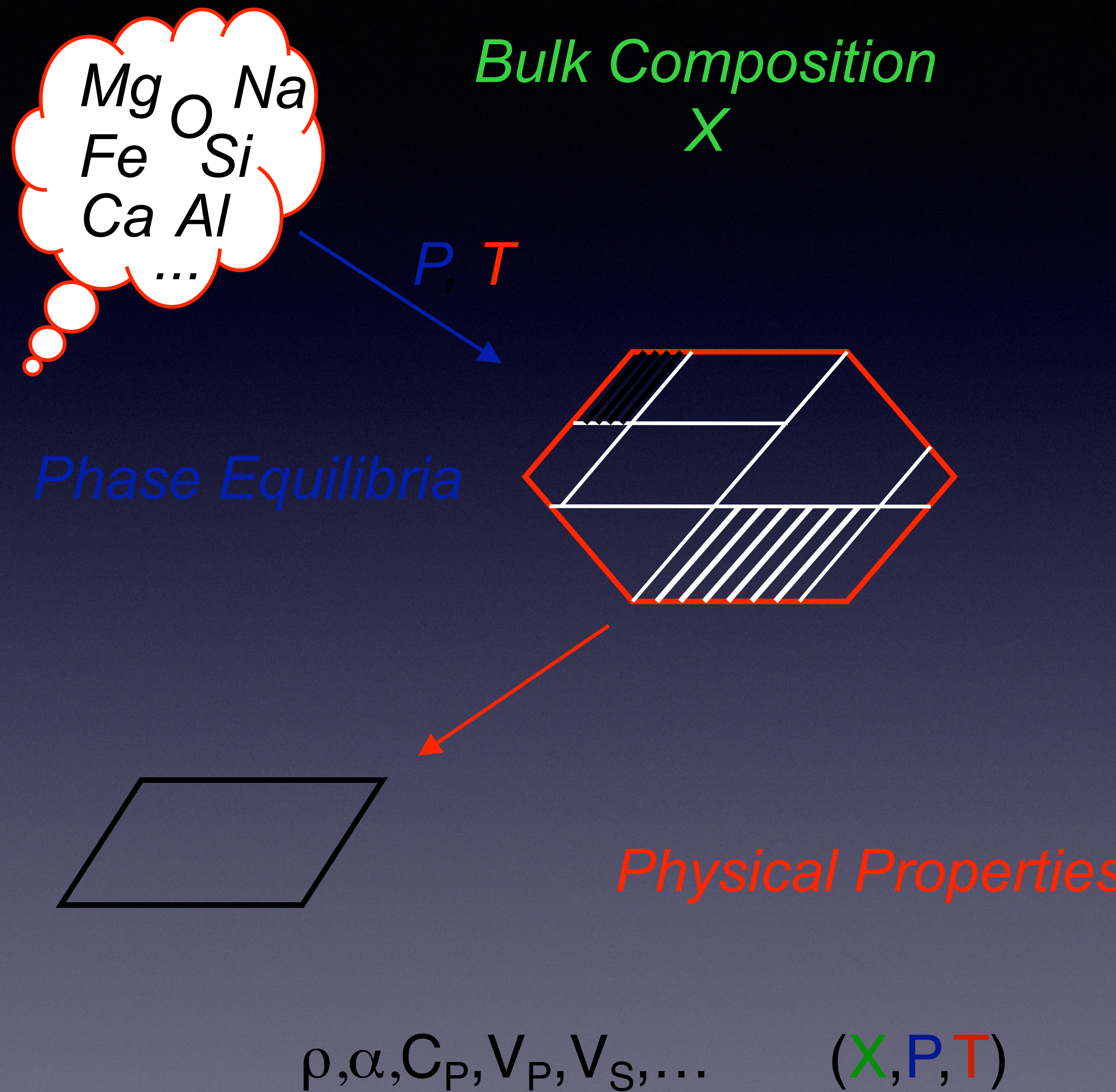


Stixrude and Lithgow-Bertelloni 2007

Thermodynamic Model

- Bulk composition
- Pressure
- Temperature

- Phase Equilibria
- Physical Properties
- Self consistent



Stixrude and Lithgow-Bertelloni 2005

HeFESTo

- Based on Fundamental Thermodynamic Relations
- Minimize Gibbs free energy over the amounts of all species n_i

$$G(P,T,n_i) = \sum_{i=1}^{species} n_i\left[\mu_{0i}(P,T) + RT\ln a_i\right]$$

- Subject to constraint of fixed bulk composition

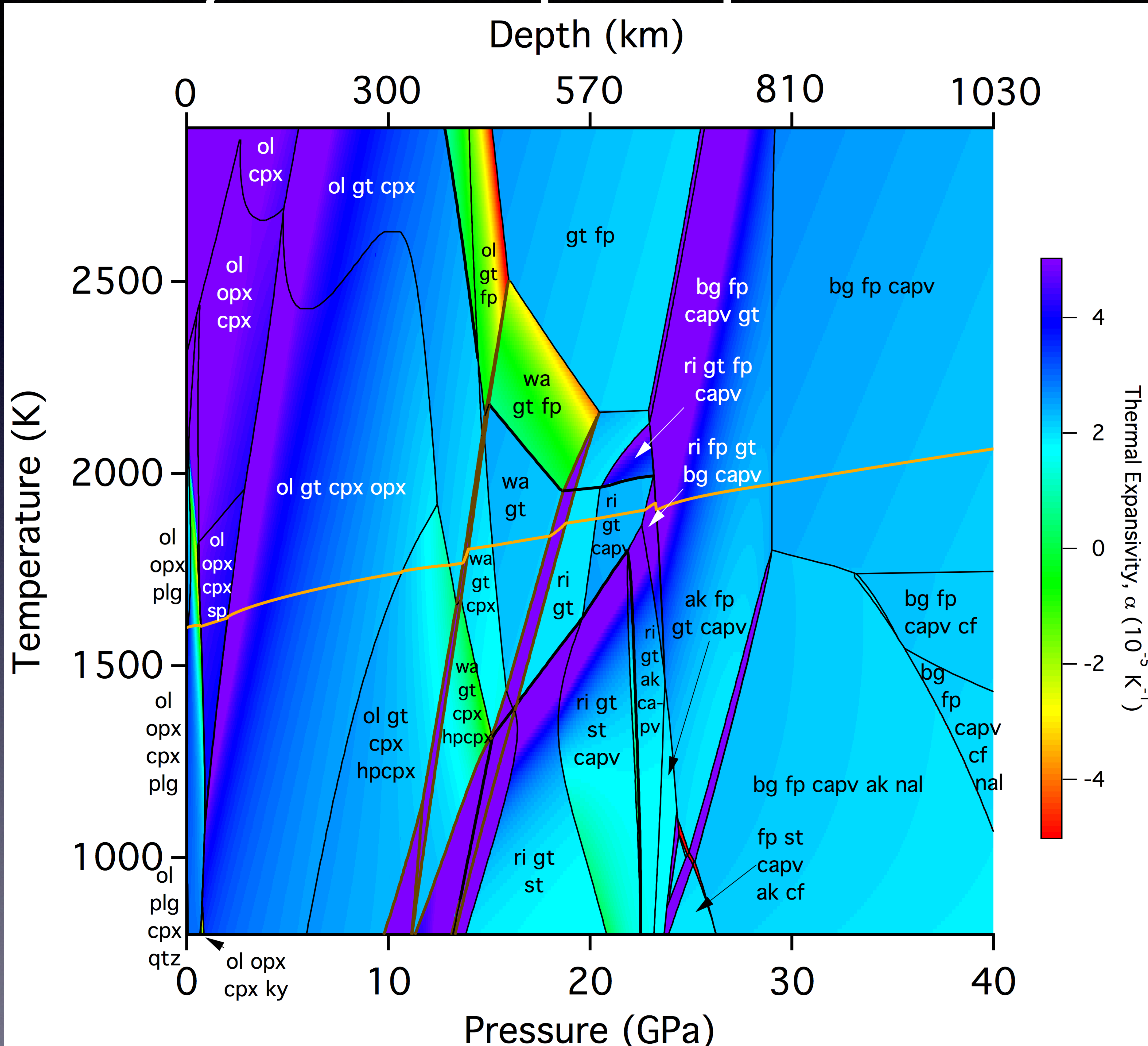
$$s_{ij}n_j = b_i$$

- Full Anisotropic Generalization

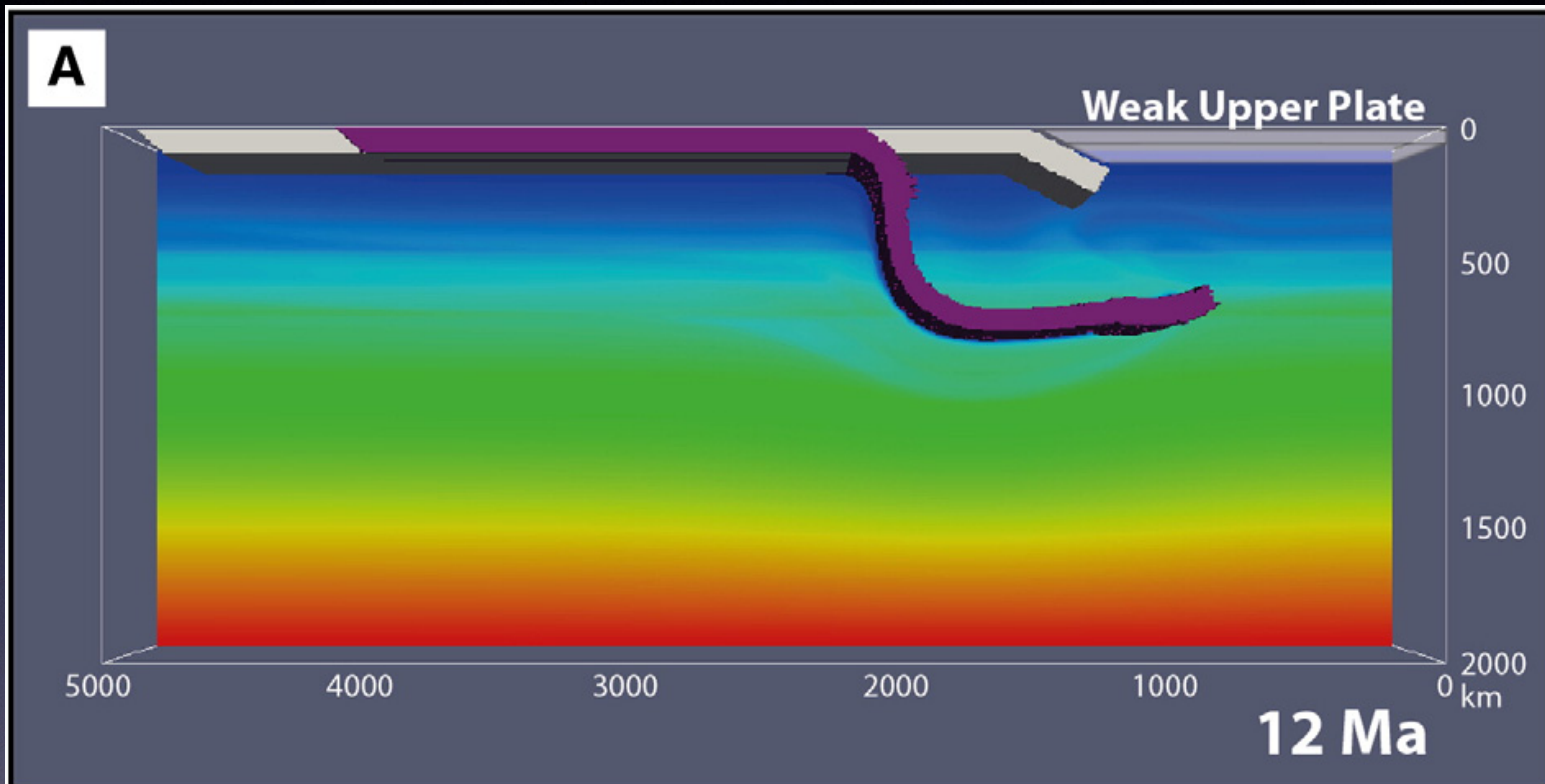
$$c_{ijkl} = \frac{1}{V}\left(\frac{\partial^2 F}{\partial E_{ij}\partial E_{kl}}\right)_{S'_{ij},T} + P\left(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik}\right)$$

- Many previous efforts, however
  - Full self-consistency between phase equilibria and physical properties (not only one or the other)
  - Anisotropic generalization and robust thermal extrapolation for shear properties

Physical properties



Importance for flow

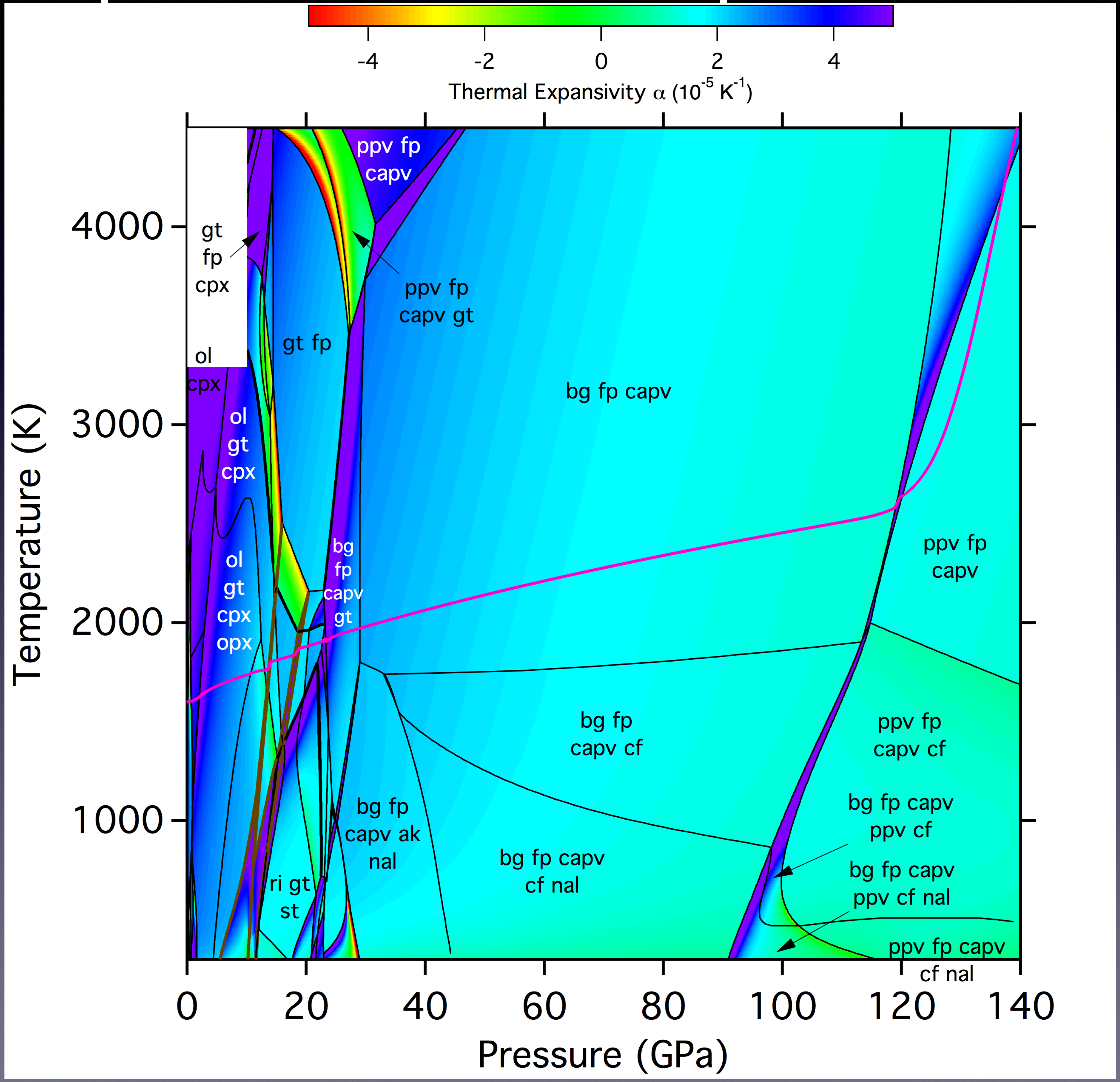


Faccenda and Dal Zilio 2016

So does including full thermodynamics matter?

- Nakagawa et al. (2009)
- not much difference… not much induced layering for today’s conditions
- But has this always been the case? (i.e. Allégre, 1997)
- If not, could there have been layering and help preserve heterogeneity as geochemistry suggests?
- Mass transfer may be recent (~ 1 Ga)
- Transition caused by cooling and reduction in Ra

Temperature Dependence

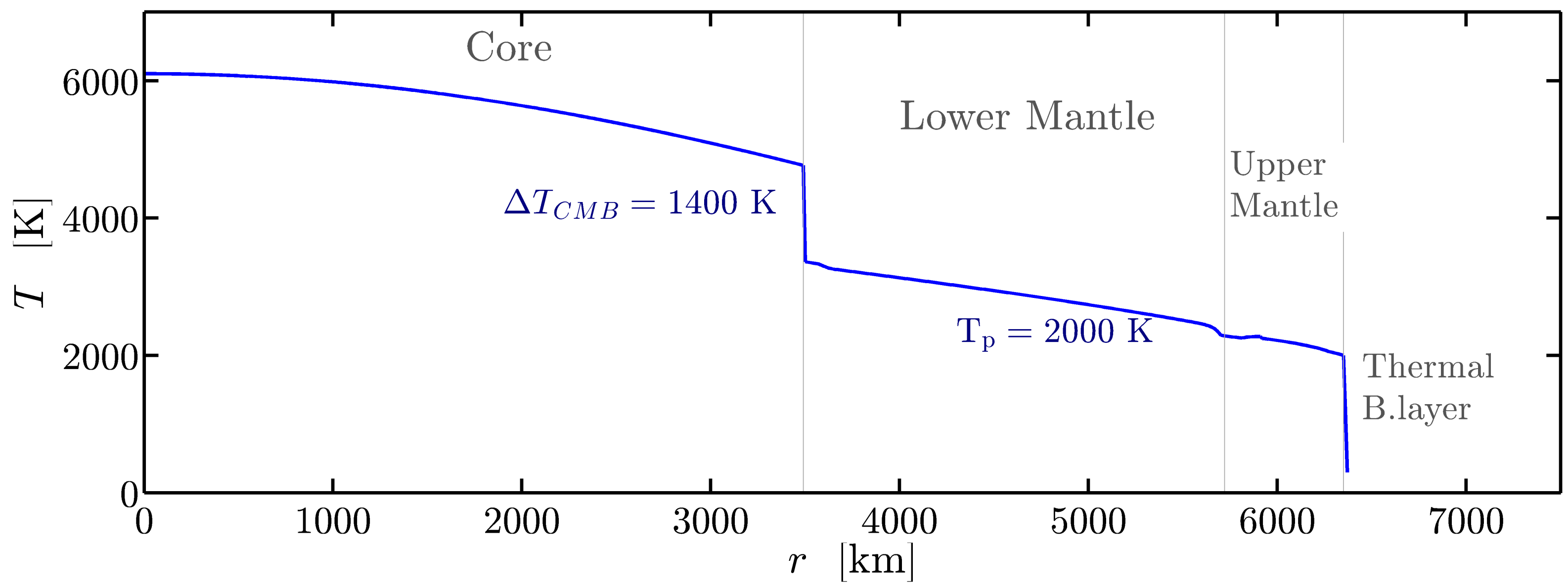


1-D temporal evolution

- 1D model of Earth (post-magma ocean)
- Examine thermal evolution of mantle and core
- Uses Hefesto to calculate mantle properties
- Model Tracks
    - State Variables (T(K) and P (Pa)
    - ρ, α, C_p from Hefesto
    - Thermal conductivity, k_c [W/m K] (5-10 for mantle, 40 for core) Viscosity, μ [Pa s] (Arrhenius form, with activation energy, volume and other constants from Ranalli, 2001)
- Core equation of state by fitting to PREM

Initial Conditions

Initial temperature profile



Adiabatic in core and mantle:

$$\frac{\partial T}{\partial r} = \left(\frac{\partial T}{\partial r}\right)_S = -T\left(\frac{\alpha g}{C_p}\right)$$

- Find initial state by iterating on P, g, T, ρ, α, etc.

Temperature Evolution- Mixing Length theory

Energy equation

$$\frac{\partial}{\partial t}(\rho C_p T) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k_c \frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k_v \left[\left(\frac{\partial T}{\partial r}\right) - \left(\frac{\partial T}{\partial r}\right)_S\right]^2\right) + \rho Q$$

To model in 1D, need to parameterise convection:

$$k_v = \begin{cases} \frac{\rho^2 C_p g \alpha \ell^4}{18\mu}, & \text{if } \left(\frac{\partial T}{\partial r}\right) < \left(\frac{\partial T}{\partial r}\right)_S \\ 0, & \text{otherwise,} \end{cases}$$

No convection if sub-adiabatic.

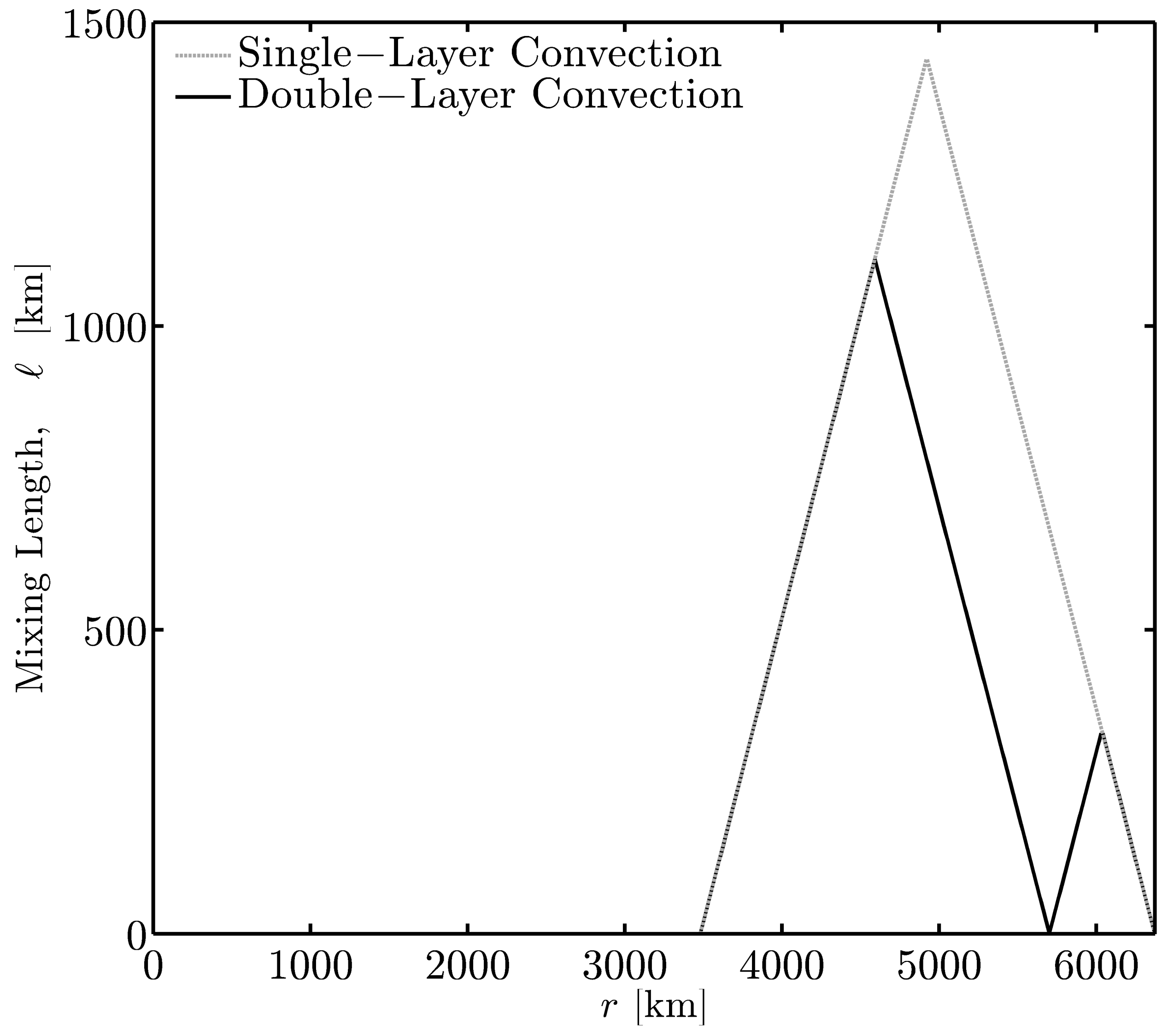
In uniform cartesian flow this is equivalent to:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + Ra \frac{\partial}{\partial x}\left(\ell^4 \left(\frac{\partial T}{\partial x}\right)^2\right) + \frac{Ra_Q}{Ra}$$

Kimura et al 2009

Thermal Evolution in the Mantle

- Strength of convection depends strongly on mixing length, ℓ
- Set ℓ to distance to nearest boundary of fluid layer
- Can have single- or double-layer convection



- Allow ℓ to vary dynamically according to local flow criterion -> intermittent layering

Compressible Mantle

Need to account for compressibility

Energy equation solves for $\frac{\partial}{\partial t}(\rho C_p T)$, not $\frac{\partial T}{\partial t}$

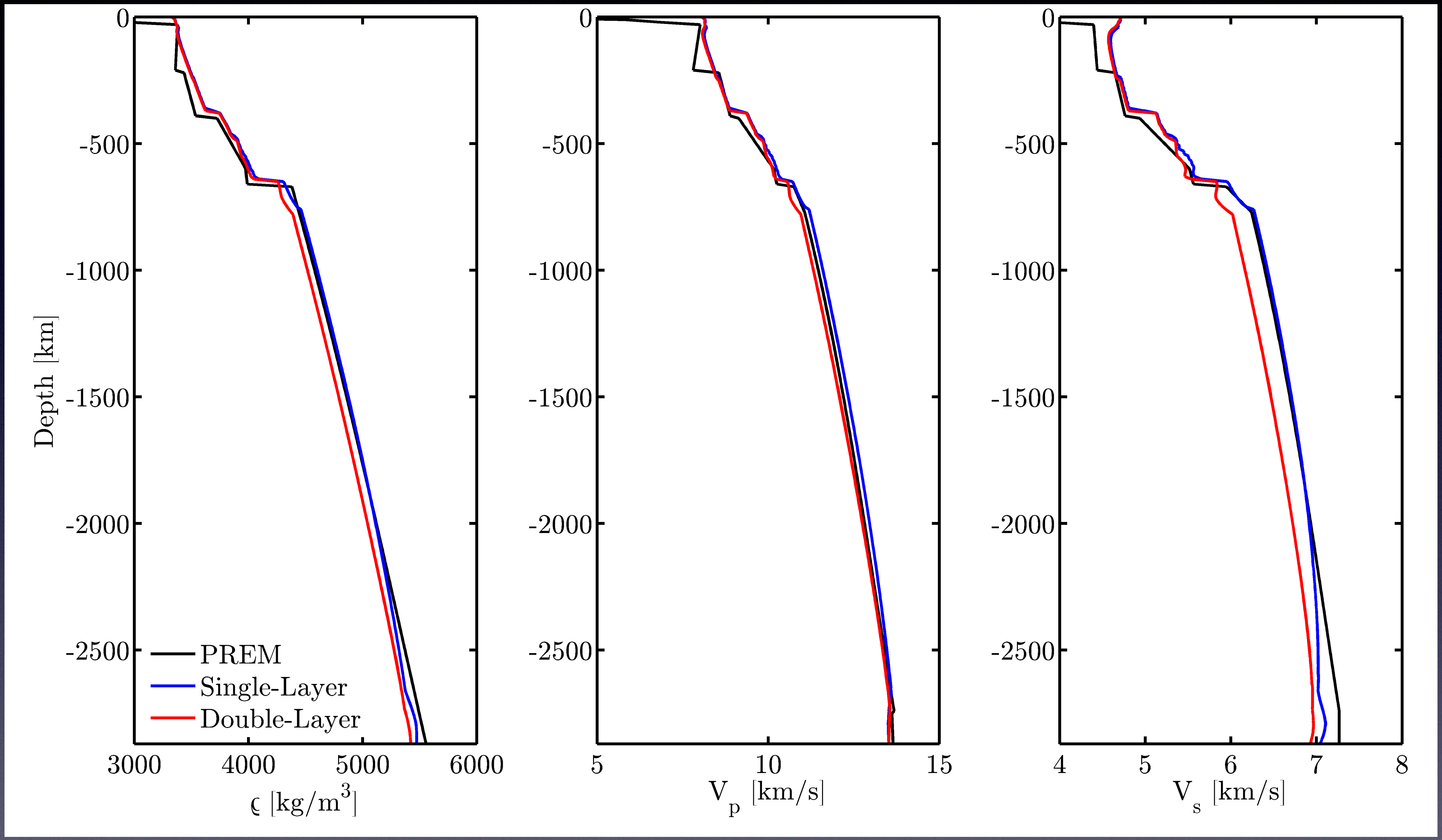
Simple differentiation:

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho C_p T) &= \rho C_p \frac{\partial T}{\partial t} + T\frac{\partial \rho C_p}{\partial t} \\
&= \rho C_p \frac{\partial T}{\partial t} + T\frac{\partial \rho C_p}{\partial T}\frac{\partial T}{\partial t} \\
&= \left(\rho C_p + T\frac{\partial \rho C_p}{\partial T}\right)\frac{\partial T}{\partial t} \\
&= \beta(T,P)\frac{\partial T}{\partial t}.
\end{aligned}$$

$\beta(T,P)$ can be found from Hefesto data

Some validation

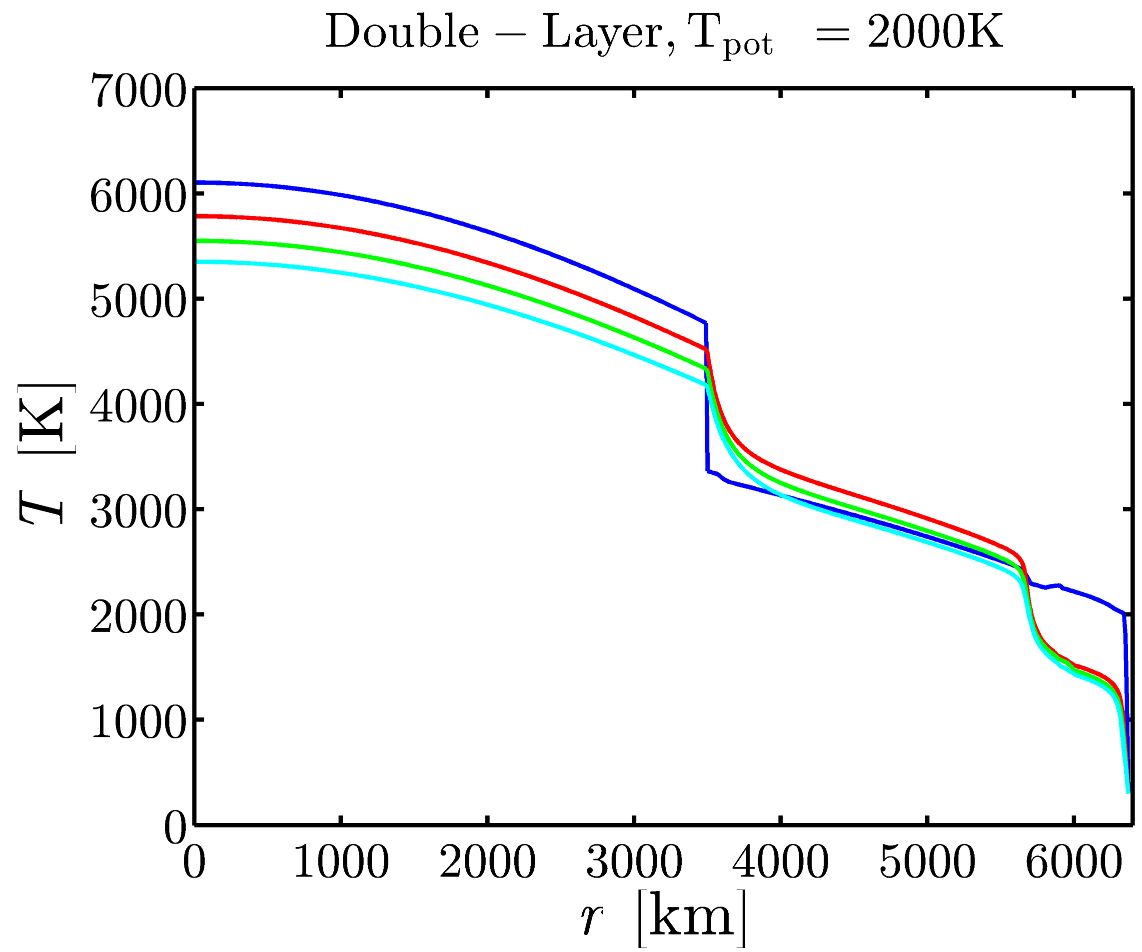
- For initial T_p = 2000 K



- $r = 1 - 6371$, with $\Delta r = 10$ km
- Maximum ΔT per timestep is 0.1 K
  (average $\Delta t \approx 10^4$ years)
- 2nd order Runge-Kutta
- Three cases (choice of ℓ):
  single-layer, double-layer and intermittently layered

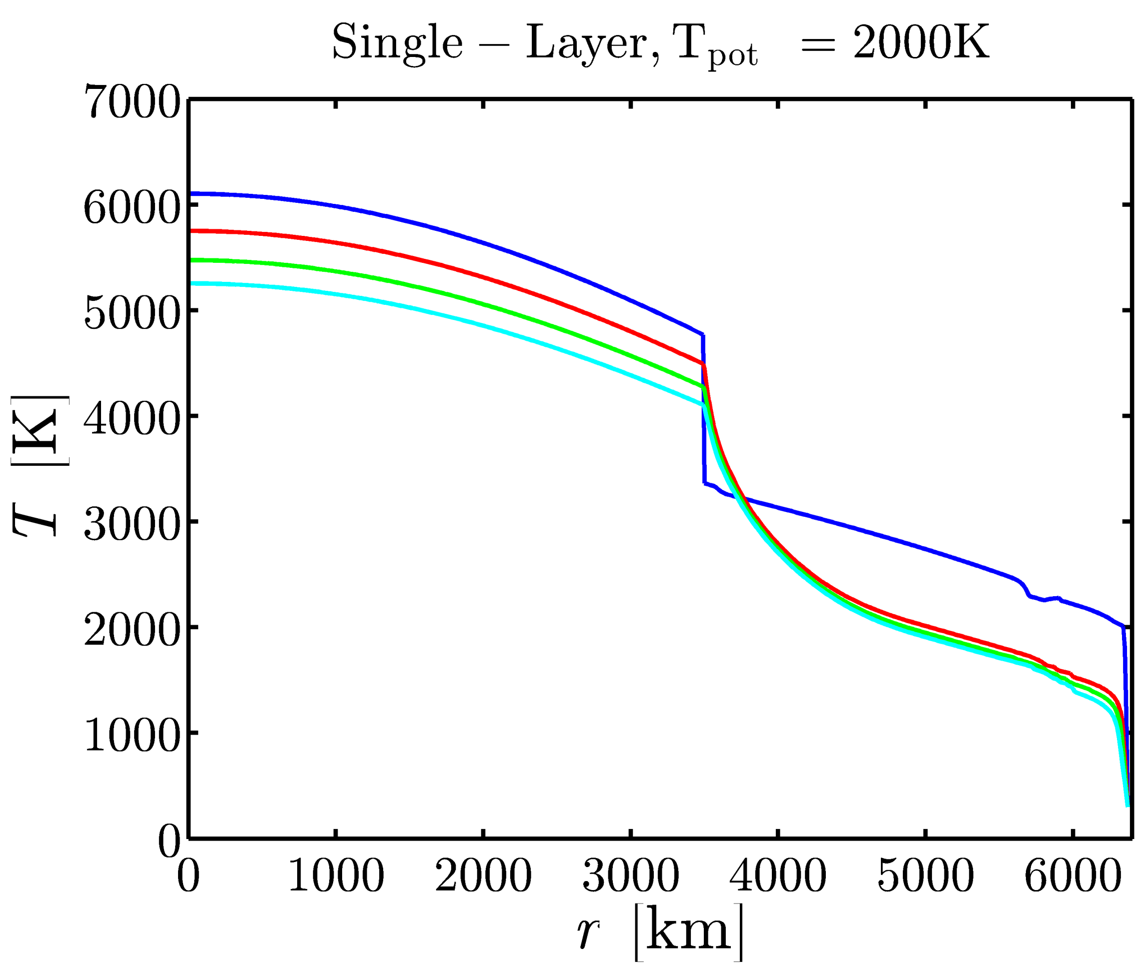
- Q_{CMB} ~ 7 TW (estimated 5±5)
- Q_S ~ 35 TW (estimated 47)

Evolution

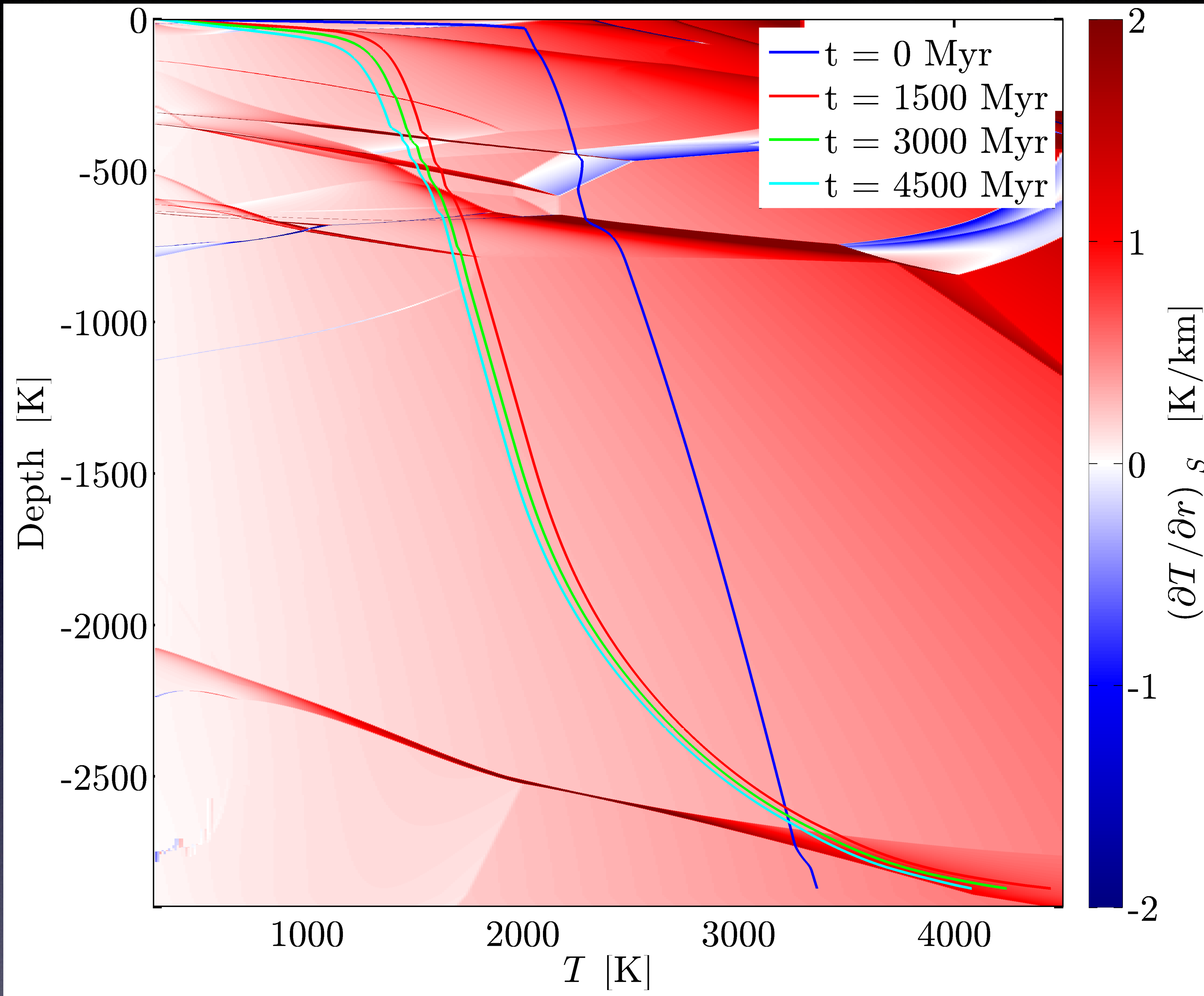


- Upper mantle cools rapidly
- Lower mantle remains insulated
- Heats up due to radiogenic heating

- Quickly reaches steady-state
- Consequence of Arrhenius rheology

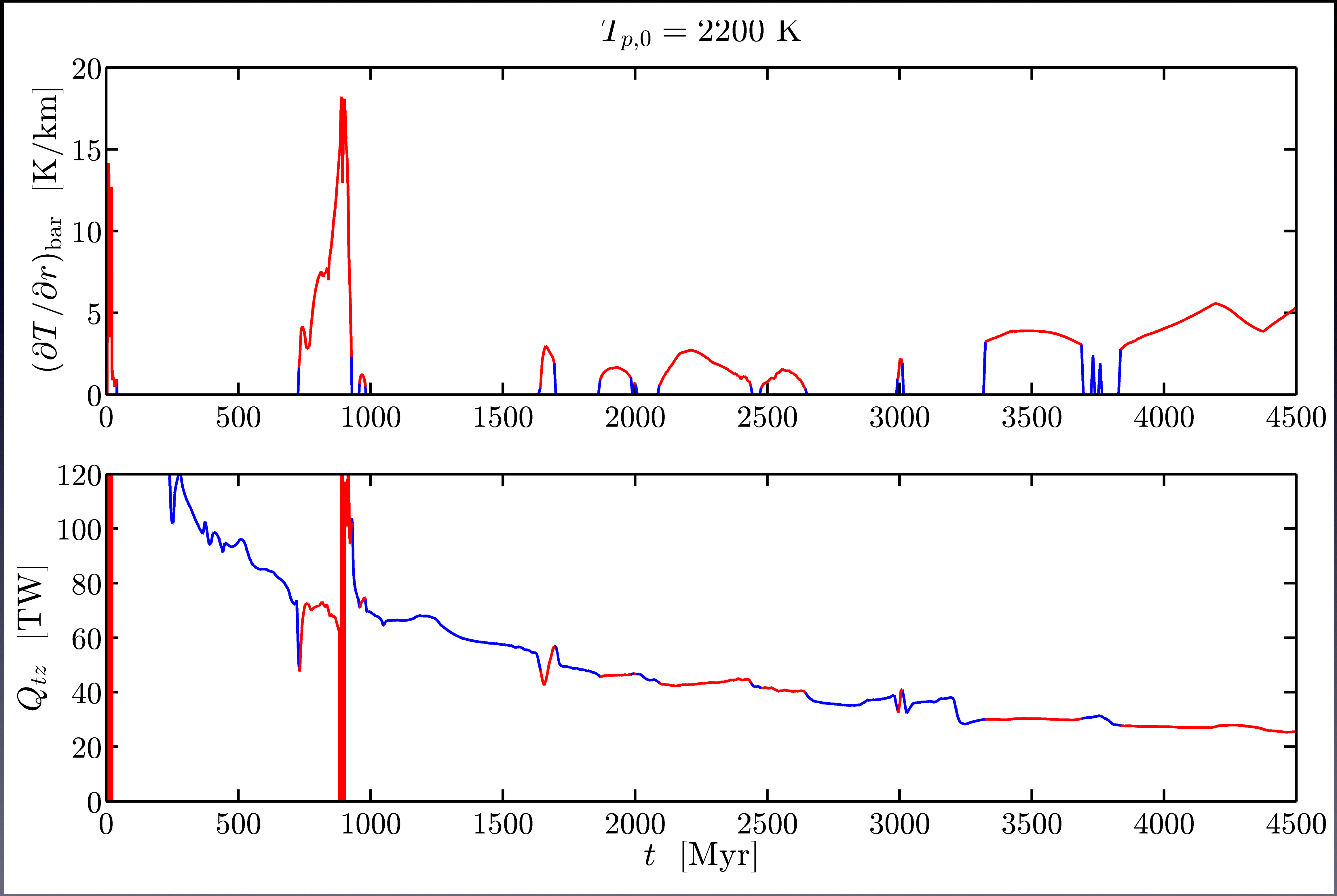


Evolution



- As mantle cools, geotherm passes through regions of different $(\partial T/\partial r)_S$
- Can prevent convection if $(\partial T/\partial r)_S \lesssim -2$ K/km, or > 0
- Ability to convect heat across transition zone will vary with time

Intermittent Layering



- Layered state about ~80% of the time

Results

- Layering arises naturally from thermodynamics
- Doesn't depend on Ra
- Layering can preserve chemical reservoirs in lower mantle
- Some plumes may 'push through' despite being sub-adiabatic

How can we estimate effect of layering on heterogeneity preservation?

- Understanding effect of layering on chemical reservoirs requires information on isotopic flux

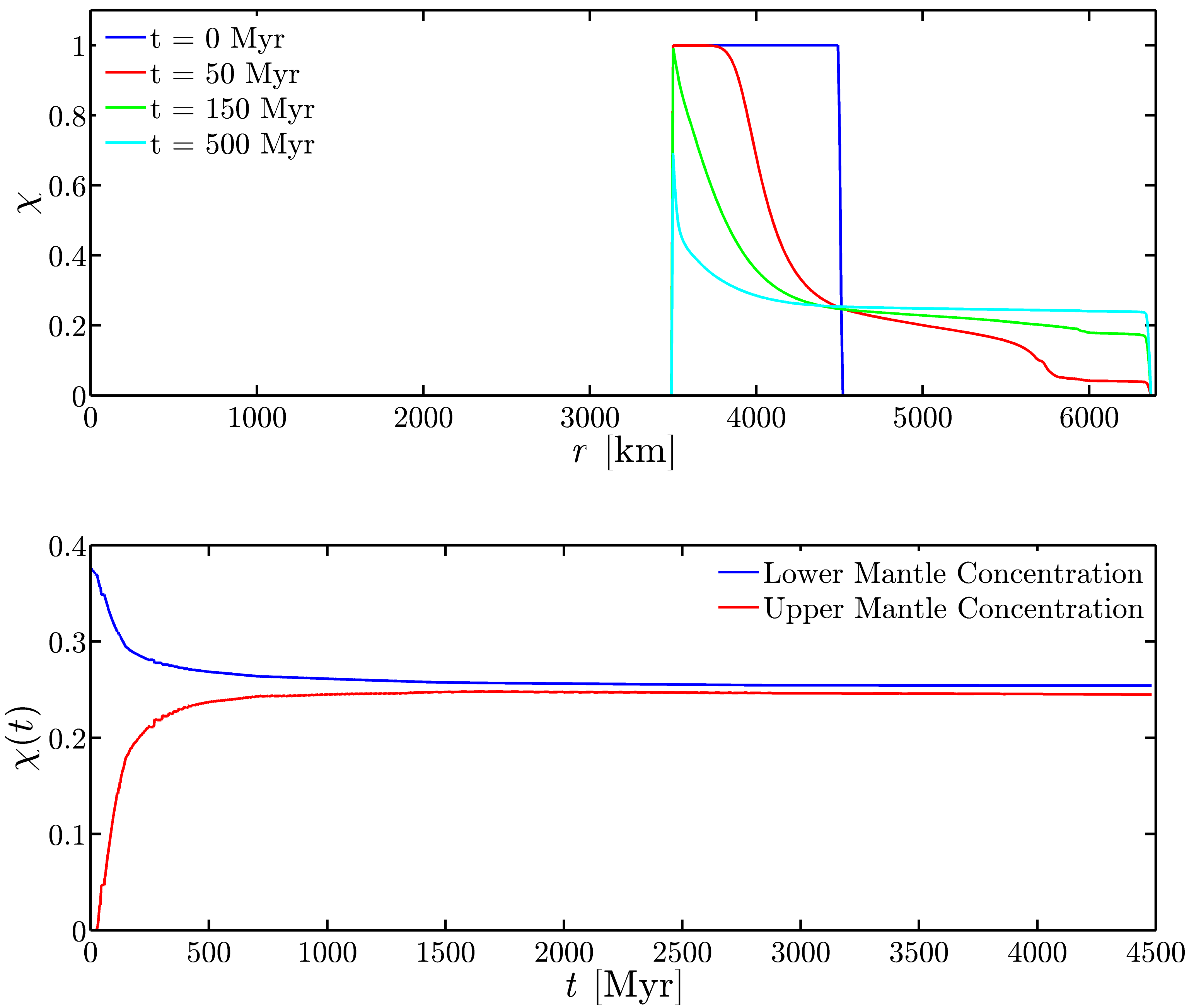
- Can estimate using MLT:

$$\frac{\partial \chi}{\partial t} = \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left(\frac{r^2 \rho^2 C_p \alpha g \left[\left(\frac{\partial T}{\partial r} \right) - \left(\frac{\partial T}{\partial r} \right)_S \right] \frac{\partial \chi}{\partial r} \ell^4}{18\mu} \right)$$

How can we estimate effect of layering on heterogeneity preservation?

Can use $\partial \chi / \partial t$ to investigate:

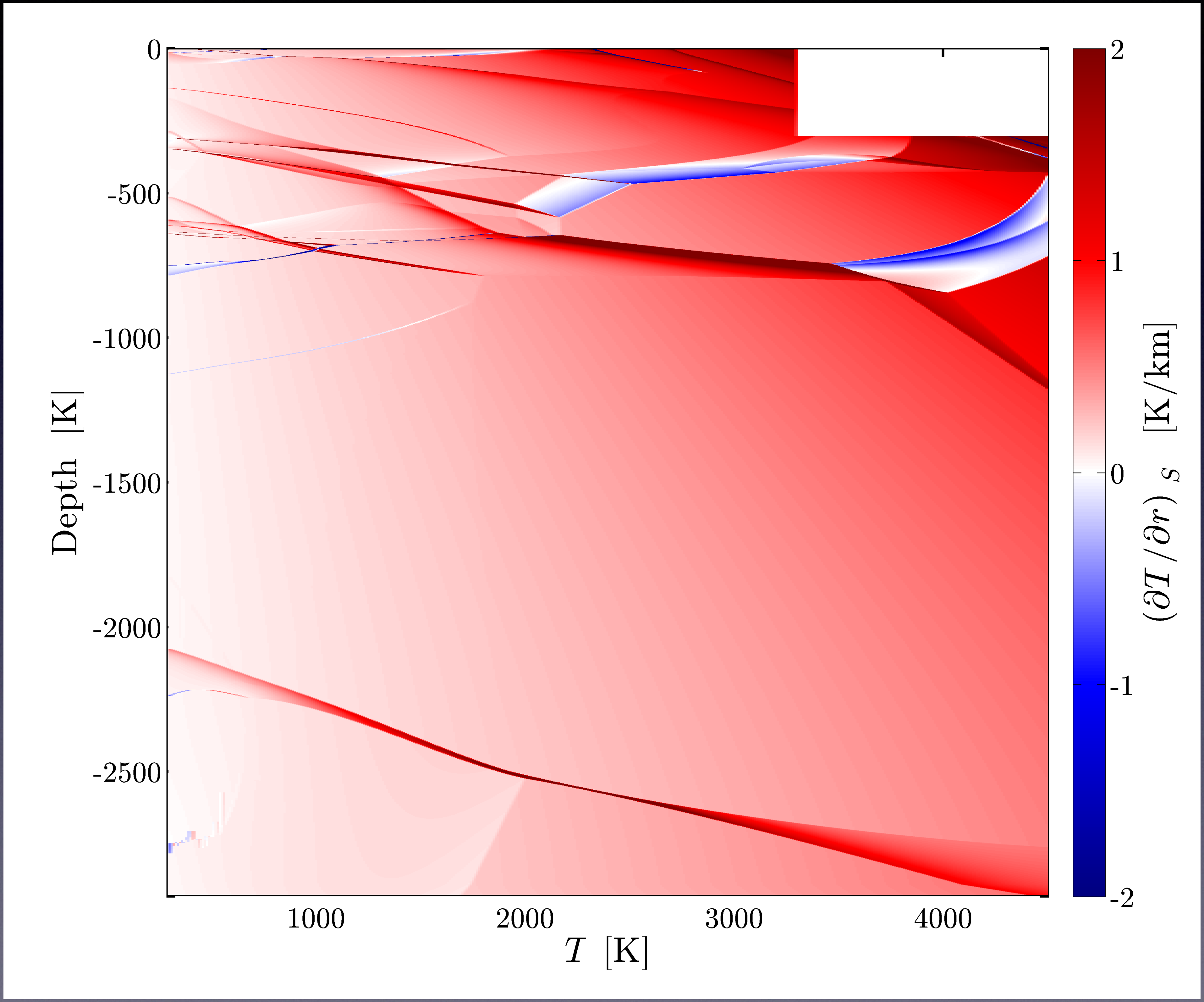
- Mixing times
- Variation in bulk composition of mantle (e.g. proportion of depleted mantle)
- Volatile flux (effect of water-dependent rheology)



Conclusions and Future Goals

- Explore mass transfer evolution
- 3D convection with full thermo with secular cooling
    - Important to capture very sharp phase transitions
    - Adaptivity (i.e. ASPECT, Fluidity essential)
- Implications for Earth's geochemical evolution

Sharp Transitions



Mixing Length Theory

Theory outlined in Kimura et al. Size and compositional constraints of Ganymede's metallic core for driving an active dynamo, *Icarus*, 202, 216-224, 2009.

$$\frac{\partial}{\partial t}\left(\rho C_p T\right) = \nabla \cdot q'' + H$$
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k_c \frac{\partial T}{\partial r}\right) + \nabla \cdot q_v'' + H$$

For convection, $q_v'' \approx \rho C_p \Delta T U$

Assume U is stokes velocity

$$U = \frac{2\Delta\rho g(\ell/2)^2}{9\mu} = \frac{\Delta\rho g \ell^2}{18\mu}$$

Where

$$\Delta\rho = \rho\alpha\Delta T$$

$$\Delta T = \left[\left(\frac{\partial T}{\partial r}\right) - \left(\frac{\partial T}{\partial r}\right)_S\right]\ell$$

Combining, U, $\Delta\rho$, ΔT.

$$q_v'' = \frac{\rho^2 C_p \alpha g \left[\left(\frac{\partial T}{\partial r}\right) - \left(\frac{\partial T}{\partial r}\right)_S\right]^2 \ell^4}{18\mu}$$

Mixing Length Theory: Mass flux

Conservation of mass

$$\frac{\partial}{\partial t}(\rho\chi) = \nabla \cdot \dot{m}$$

For convection,

$$\begin{aligned}\dot{m} &\approx \rho\,(\Delta\chi)\,U \\ &\approx \rho\left(\frac{\partial\chi}{\partial r}\ell\right)U\end{aligned}$$

Again, U is stokes velocity

$$U = \frac{\Delta\rho g \ell^2}{18\mu} = \frac{\rho\alpha\left[\left(\frac{\partial T}{\partial r}\right) - \left(\frac{\partial T}{\partial r}\right)_S\right]\ell^3}{18\mu}$$

Combining, we get

$$\dot{m} = \frac{\rho^2 C_p \alpha g\left[\left(\frac{\partial T}{\partial r}\right) - \left(\frac{\partial T}{\partial r}\right)_S\right]\frac{\partial\chi}{\partial r}\ell^4}{18\mu}$$

Physical properties